

XY ring exchange model with frustrated Ising coupling on the triangular lattice

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Abstract

We investigate the nature of a Z_2 -invariant XY ring-exchange interaction with a frustrated Ising coupling on the triangular lattice. In the limit of pure XY ring-exchange interaction, we show that the classical ground state is degenerate resulting from the Z_2 -invariance of the Hamiltonian. Quantum fluctuations lift these classical degenerate ground states and produce an unusual state whose excitation spectrum exhibits a gapped maximum quadratic dispersion near $\mathbf{k} = 0$ and vanishes at the midpoints of each side of the Brillouin zone. This result is in contrast to a gapless quadratic dispersion near $\mathbf{k} = 0$ in the U(1)-invariant counterpart. We also study the effects of frustration when competing with a classically frustrated Ising interaction. We provide a glimpse into the possible quantum phases that could emerge. A comprehensive understanding of this Hamiltonian, however, cannot be elucidated analytically and requires an explicit numerical simulation.

1. Introduction

The study of quantum spin ice (QSI) on three dimensional (3D) pyrochlore lattice has attracted considerable attention [1–13]. Huang-Chen-Hermele [1] have proposed an alternative Hamiltonian for QSI in 3D pyrochlore lattice, applicable to certain class of d - and f -electron systems with dipolar-octupolar Kramers doublets. Using dimensional reduction [10–12], Carrasquilla *et al.*, [2] have recently mapped this model to 2D kagome lattice with a [111] crystallographic field. They have identified the interaction that promotes a putative quantum spin liquid (QSL) state and uncovered the low-temperature quantum phase diagram using a non-perturbative, unbiased QMC simulations on the kagome lattice [2]. In this system, competition between the classical Ising frustration and a Z_2 -invariant ferromagnetic quantum fluctuation lead to a putative QSL state. Thus, there is a possibility to search for 2D QSL states within a class of pyrochlore quantum spin ice materials. The distinctive feature of the QSI Hamiltonian is the presence of Z_2 symmetry. We have recently studied the 2D quantum kagome ice Hamiltonian of Carrasquilla *et al.*, [2] on the triangular lattice [14], using spin wave theory. An explicit numerical simulation has not been reported at the moment. However, spin wave theory still captures the interesting properties of the system because quantum fluctuations are suppressed in this model. In principle, there is a possibility of a ring exchange interaction that exhibits a Z_2 symmetry, as in the U(1)-invariant XY model (hard-core bosons) with ring-exchange interactions [15–26]. The ring exchange quantum spin Hamiltonian is believed to be very important in Wigner crystals near the melting density [27–29]. They also promote interesting quantum properties with rich quantum phase diagram.

In this communication, we consider the competing interactions between a classically frustrated Ising interaction and a Z_2 -invariant ring exchange interaction. The Hamiltonian can be written as

$$H = J_z \sum_{\langle ij \rangle} S_i^z S_j^z + K \sum_{\langle ijkl \rangle} (S_i^+ S_j^+ S_k^+ S_l^+ + S_i^- S_j^- S_k^- S_l^-), \quad (1)$$

where $S_l^\pm = S_l^x \pm iS_l^y$ are the raising and the lowering spin operators respectively. A special feature of this Hamiltonian is that it exhibits only Z_2 -symmetry in the x - y plane, *i.e.*, π -rotation about the z -axis in spin space, $S_\mu^\pm \rightarrow -S_\mu^\pm$, $S_\mu^z \rightarrow S_\mu^z$; $\mu = i, j, k, l$. The Hamiltonian (Eq. (1)) can be studied in any lattice geometry. However, for bipartite lattices, Eq. (1) is related to a U(1)-invariant model by a π -rotation about the x -axis on two sublattices, *i.e.*, $S_{i,j}^\pm \rightarrow S_{i,j}^\mp$; $S_{i,j}^z \rightarrow -S_{i,j}^z$. We restrict our analyses to the triangular lattice. Hence, the summation over the ring exchange term runs over the three possible four-spin plaquette orientations on a triangular lattice; see Fig. (1). We will investigate the distinctive features of the pure Z_2 -invariant XY ring-exchange Hamiltonian ($J_z = 0$) and its effects when competing with a classical Ising frustration ($J_z < K$, with $K < 0$). The study of this Hamiltonian is partially motivated by the quantum phases uncovered in 2D QSI Hamiltonian [2] and the recent study of the 2D QSI Hamiltonian on the triangular lattice [14].

2. Pure-K model

In order to get an insight into the effects of Z_2 symmetry of Eq. (1), we consider the pure- K model in Eq. (1), which corresponds to $J_z = 0$. In this limit, the resulting Hamiltonian has a related U(1)-invariant counterpart [18, 19]. The important feature of the U(1)-invariant pure- K model is that the energy spectra has a gapless quadratic excitation near $\mathbf{k} = 0$ [18–20].

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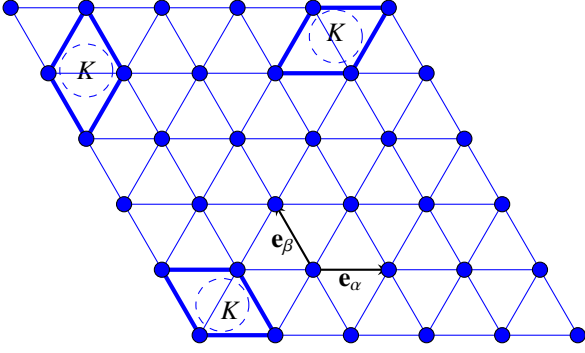


Figure 1: Color online. Triangular lattice with three-plaquette orientations (thick lines). The ring exchange interaction acts on the four sites within each plaquette. \mathbf{e}_α and \mathbf{e}_β are the primitive vectors on the triangular lattice.

However, the present model is devoid of continuous symmetries. The behaviour of the excitation spectra is not known in literatures. It is interesting to investigate how the excitations behave in the long wavelength limit. The Hamiltonian, Eq. (1), in this limit ($J_z = 0$) can be written explicitly as

$$H_{J_z=0} = 2K \sum_{\langle ijkl \rangle} \left(S_i^x S_j^x S_k^x S_l^x + S_i^y S_j^y S_k^y S_l^y \right. \\ \left. - S_i^x S_j^y S_k^x S_l^y - S_i^y S_j^x S_k^y S_l^x - S_i^x S_j^x S_k^y S_l^y \right. \\ \left. - S_i^y S_j^y S_k^x S_l^x - S_i^x S_j^y S_k^y S_l^x - S_i^y S_j^x S_k^x S_l^y \right). \quad (2)$$

Classically, the ground state of Eq. (2) is highly degenerate resulting from the Z_2 symmetry of the Hamiltonian. The ground state corresponds to all possible spin configurations along the basis \mathbf{e}_α and \mathbf{e}_β (see Fig. (1)), and it is independent of the sign of K . There are several ways to investigate how quantum fluctuations select a particular classical ground state in this system. In the U(1)-invariant model, this can be done by integrating out the phase fluctuations about the classical ground state in the path integral for the partition function [18]. This method, however, is effectively the same as performing spin wave theory about any classical ground state of Eq. (2). The collective excitation spectrum is the same in both methods.

Since we have only x - y coupling in Eq. (2), one can show that the excitation spectrum about any classical ground state is the same, provided one rotates the axes properly. In the present model there is no conserved quantity, it is expedient to use a direct spin wave theory via the Holstein Primakoff transform [30]. We choose the easy-axis ferromagnetic state, and implement the linearized Holstein Primakoff transformation, [30, 31]

$$S_j^x = S - b_j^\dagger b_j, \quad S_j^y = i\sqrt{\frac{S}{2}} (b_j^\dagger - b_j). \quad (3)$$

Next, we restrict the spins to $S = 1/2$, substitute Eq. (3) into Eq. (2) and Fourier transform over the three plaquettes. The resulting bosonic Hamiltonian is very lengthy to write here. It can be diagonalized by the Bogoliubov transformation,

$$b_{\mathbf{k}} = u_{\mathbf{k}} \gamma_{\mathbf{k}} - v_{\mathbf{k}} \gamma_{-\mathbf{k}}^\dagger, \quad (4)$$

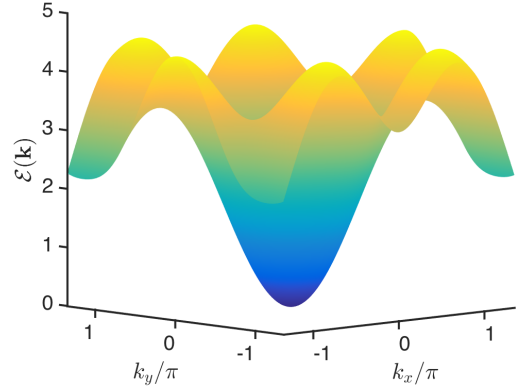


Figure 2: Color online. The spin wave excitation spectrum of the U(1)-invariant pure- K model. The coupling is set to unity.

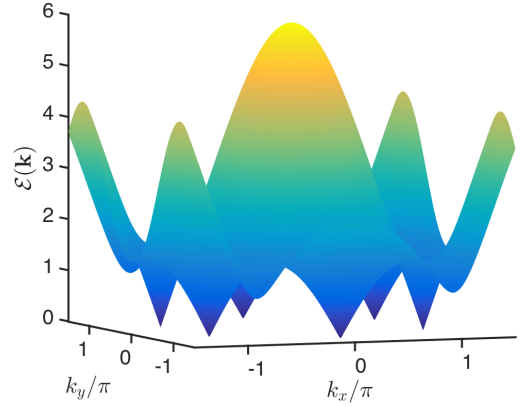


Figure 3: Color online. The energy dispersion of the Z_2 -invariant pure- K model. The coupling is set to unity. Fig. (4) shows the points where the energy vanishes.

where $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$, one finds that the resulting Hamiltonian is diagonalized by

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left(\frac{A_{\mathbf{k}}}{E_{\mathbf{k}}} + 1 \right); \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left(\frac{A_{\mathbf{k}}}{E_{\mathbf{k}}} - 1 \right), \quad (5)$$

with $E_{\mathbf{k}} = \sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}$.

The diagonal Hamiltonian yields

$$H_{J_z=0} = \sum_{\mathbf{k}} E_{\mathbf{k}} (\gamma_{\mathbf{k}}^\dagger \gamma_{\mathbf{k}} + \gamma_{-\mathbf{k}}^\dagger \gamma_{-\mathbf{k}}). \quad (6)$$

The excitation of the quasiparticles is given by

$$\mathcal{E}(\mathbf{k}) = 2E_{\mathbf{k}} = 2\sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}, \quad (7)$$

$$A_{\mathbf{k}} = \frac{3K}{2} - B_{\mathbf{k}}, \quad B_{\mathbf{k}} = -\frac{K}{2} \lambda_{\mathbf{k}} - \frac{K}{8} (\lambda_{\mathbf{k}} + \bar{\lambda}_{\mathbf{k}}), \quad (8)$$

and

$$\lambda_{\mathbf{k}} = \cos k_\alpha + \cos k_\beta + \cos(k_\alpha + k_\beta); \quad (9)$$

$$\bar{\lambda}_{\mathbf{k}} = \cos(k_\alpha - k_\beta) + \cos(2k_\alpha + k_\beta) + \cos(k_\alpha + 2k_\beta). \quad (10)$$

where $k_\alpha = \mathbf{k} \cdot \mathbf{e}_\alpha$ and $k_\beta = \mathbf{k} \cdot \mathbf{e}_\beta$.

In Fig. (2) we have shown the spin wave spectrum of the $U(1)$ -invariant model obtained in Ref. [18] using a different approach. In this case, there is one quadratic gapless mode at $\mathbf{k} = 0$. In contrast, Fig. (3) shows the spin wave spectrum for the present model. We observe instabilities of the spin wave at the midpoints of the adjacent sides of the Brillouin zone, that is at the points A , B , and C in Fig. (4). At the center of the Brillouin zone the spectrum exhibits a gapped maximum dispersion, which in the long wavelength limit behaves as

$$\mathcal{E}(\mathbf{k}) = a - b|\mathbf{k}|^2, \quad (11)$$

where $a = 6K$ and $b = 3K/4$. The maximum dispersion near

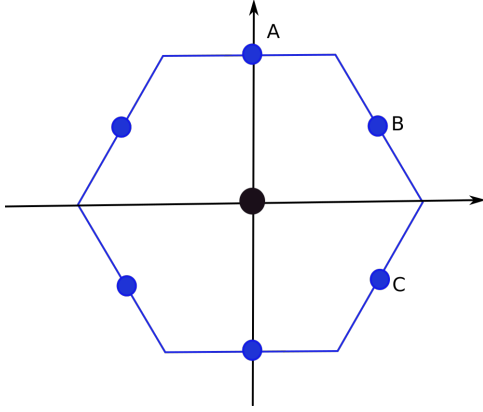


Figure 4: Color online. The Brillouin zone of the triangular lattice. The points A , B , and C are the midpoints of the adjacent sides of the Brillouin zone, where the energy vanishes.

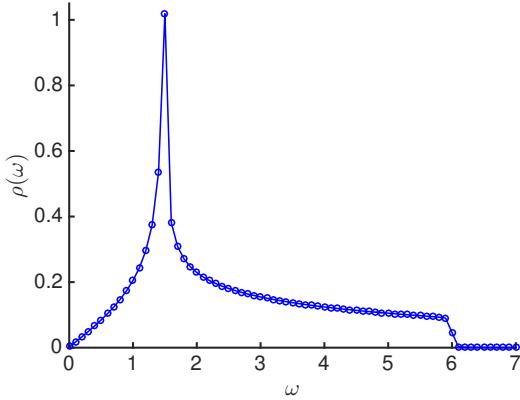


Figure 5: Color online. The density of states, $\rho(\omega)$, of the Z_2 -invariant pure- K model.

$\mathbf{k} = 0$ is one of the distinctive features of this model as a result of pure Z_2 symmetry of the Hamiltonian.

Figure (5) shows the plot of the density of states for the pure- K model, given by

$$\rho(\omega) = \frac{1}{V} \sum_{\mathbf{k}} \delta(\omega - \mathcal{E}(\mathbf{k})). \quad (12)$$

The distinguishing feature of the density of states is that the largest peak correspond to the saddle point of the excitation energy. The maximum excitation energy, however, is at much higher energy and leads to a step-like van Hove singularity. The density of states also shows a discontinuity corresponding to the vanishing of the excitation spectrum at the midpoints of adjacent sides of the Brillouin zone in Fig. (3). Thus, the Z_2 -invariant pure- K model describes an unusual liquid.

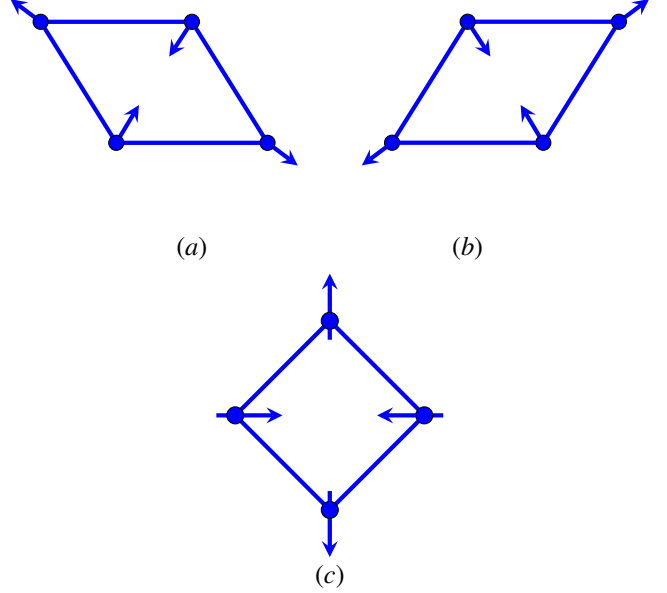


Figure 6: Color online. The spin configurations on the triangular plaquettes, which obey the “ice rules” with two spins pointing inward and two spins pointing outward at each vertex.

3. Effects of frustration

We now consider the full model in Eq. (1). In the regime $J_z \ll K$, the physics of this Hamiltonian is, in fact, the same as in the previous section. In the dominant Ising coupling, $J_z > K$, the sign of K is very crucial and the system is frustrated as it is impossible to align the spins antiferromagnetically on the vertices of the triangular lattice. This leads to many classical degenerate ground states. The classical degenerate ground states of the pure- J_z term are known to be lifted through order-by-disorder mechanism [14] by quantum fluctuations emanating from the pure XY easy-axis ferromagnetic coupling $H_0 = -J \sum_{\langle ij \rangle} (S_i^+ S_j^+ + S_i^- S_j^-)$. In this case, quantum fluctuations select a particular state known as a *ferrosolid* state [14]. This state differs from the conventional *supersolid* state, [25] as it breaks translational and Z_2 symmetries.

We can imagine covering the triangular lattice with plaquettes, then one of the degenerate classical ground states of Eq. (1) obeys the ice-rules depicted in Fig. (6), in which the Ising term represents the degenerate classical ice and the ring exchange term denotes quantum fluctuations. However, the lifting of the classical degeneracy by the ring exchange term is a highly non-trivial mathematical problem. In fact, it is infeasible to analyze

this problem analytically. For $J_z > K$ and $K < 0$, there is a possibility of a gapped QSL state with gapped excitations on frustrated non-bipartite lattices. Although we cannot analytically confirm this claim, numerical techniques such as QMC should be tractable with $K < 0$. It would be interesting to investigate numerically if Eq. (1) promotes a two-dimensional QSL state within a class of triangular lattice QSL materials, [32–34] and other QSL materials on the kagome [35] and pyrochlore lattices [1–10, 13]. A related U(1)-invariant easy-axis model on the kagome lattice has been conjectured to possess a QSL phase [36].

4. Conclusion

In this communication, we presented the distinctive features of a Z_2 -invariant XY ring exchange interaction on the triangular lattice. We showed that the complete breaking of continuous U(1) symmetry down to discrete Z_2 symmetry has profound effects on the nature of the quantum properties that emerge from this system. For the pure ring-exchange model with Z_2 -invariance, we showed that the distinguishing factor is the gapped $\mathbf{k} = 0$ mode and soft modes at the midpoints of each side of the Brillouin zone. As a result, the Z_2 -invariant ring exchange model possesses some special features which are different from its U(1)-invariant counterpart. We also provided a glimpse into the nature of the possible quantum phase that could emerge when competing with a classically frustrated Ising interaction. An explicit numerical simulation is required to uncover the nature of the proposed Hamiltonian and the possibility of any two-dimensional QSL states within a class of triangular lattice QSL materials such as κ -(BEDT-TTF) $_2$ Cu $_2$ (CN) $_3$ and EtMe $_3$ Sb[Pd(dmit) $_2$] $_2$ [32–35].

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